JunLin Yu

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Education

SiChuan University Chengdu, China

Ph.D. in Pharmacy, West China School of Pharmacy 2023.9 - present
My research focus on geometric deep learning and knowledge-guided intelligent system for drug design and drug discovery.

M.S. in Pharmacy, West China School of Pharmacy 2020.9 - 2023.6
My research focus on metalloenzyme data and analysis, including traditional and deep learning-based metal-binding site identification algorithm, metalloenzyme data mining and curation, metalloenzyme-centric score function design.

B.A. in Pharmacy, West China School of Pharmacy 2016.9 - 2020.6

Research interests

Geometric Deep Learning, Generative Model; Knowledge Guidance; Physics-Inspired Biomolecule Simulation, AI4Science

Honors & Awards

2026-2027	**Doctoral Fellowship in Youth Science and Technology Talent Program**, China Association for Science and Technology	Chengdu, China
2026-2027	**Student membership**, CAAI	Chengdu, China
2025	**National Scholarship**, SiChuan University	Chengdu, China
2025	**Best Poster 1st Class**, AHeDD, ZheJiang University	Hangzhou, China
2025	**Oral presentation**, ACS Spring 2025	San Diego, US
2023	**Second Prize**, "Internet +" College Student Innovation and Entrepreneurship Competition	Chengdu, China
2023	**Outstanding Presentation Award**, National Academic Symposium for Pharmacy Graduate Students	Shenyang, China
2017	**National Encouragement Scholarship,** SiChuan University	Chengdu, China

Publications

1. **Yu, J.-L.**; et al. Knowledge-Guided Diffusion Model for 3D Ligand-Pharmacophore Mapping, ***Nat. Commun.*** 2025, 16, 2269.
2. Peng, J.*; **Yu, J.-L.***; et, al. Pharmacophore-Oriented 3D Molecular Generation towards Efficient Feature-Customized Drug Discovery. ***Nat. Comput. Sci.***, 2025.
3. **Yu, J.-L.**; et al. MeDBA: the Metalloenzyme Data Bank and Analysis platform. ***Nucleic Acids Research*** 2023, 51, D593-D602.
4. Zhang Y.-D.; **Yu, J.-L.**, et al. REaMA: Building Biomedical Relation Extraction Specialized Large Language Models Through Instruction Tuning. ***IEEE Trans. Neural Networks Learn. Syst.***, 2025.
5. **Yu, J.-L.**; et al. Geometric deep learning-enabled metal-binding site identification and grafting. ***Fundamental Research*** 2024.
6. Wu J.-W.; Ning X.-L.; Tang B.-D.; Chen Y.-T.; Yang Z.-B.; Meng F.-B.; Zhou C.; **Yu J.-L.**; et al. Deciphering Glutaminyl Cyclase Catalytic Pathways Enables Recognition of Anchor Pharmacophores for Discovering New Inhibitors. ***J. Chem. Inform. Model.*** 2025, 65, 5006–5018.
7. Zhou, C.; Cai, C.-P.; Huang, X.-T.; **Yu, J.-L.**; et al. TarKG: A Comprehensive Biomedical Knowledge Graph for Target Discovery. ***Bioinformatics*** 2024, 40.
8. **Yu, J.-L.**; et al. Advances in Computer-aided Metalloenzyme-targeted Drug Discovery. ***Chinese Journal of Modern Applied Pharmacy*** 2022, 39, 2828-2833.
9. **Yu, J.-L.**; et al. Deep learning in target prediction and drug repositioning: recent advances and challenges. ***Drug Discovery Today*** 2022.
10. Dai, Q.-Q.*; **Yu, J.-L.***; et al. Recent Advances in Deep Learning Aided Drug Discovery. ***Progress in Pharmaceutical Sciences*** 2022, 46, 60-70.
11. Yan, Y.-H.; Li, Z.-F.; Ning, X.-L.; Deng, J.; **Yu, J.-L.**; et al. Discovery of 3-Aryl Substituted Benzoxaboroles as Broad-Spectrum Inhibitors of Serine- and Metallo-β-Lactamases. ***Bioorg. Med. Chem. Lett.*** 2021, 41, 127956.
12. Xiao, Y.-C. ; **Yu, J.-L.**; et al. Targeting Metalloenzymes by Boron-Containing Metal-Binding Pharmacophores. ***J. Med. Chem.*** 2021, 64, 17706-17727.
13. Xiao, Y.-C.; Chen, X.-P.; Deng, J.; Yan, Y.-H.; Zhu, K.-R.; Li, G.; **Yu, J.-L.**; et al. Design and enantioselective synthesis of 3-(α-acrylic acid) benzoxaboroles to combat carbapenemase resistance. ***Chem. Commun.*** 2021, 57, 7709-7712.
14. Ning, X.-L.; Li, Y.-Z.; Huo, C.; Deng, J.; Gao, C.; Zhu, K.-R.; Wang, M.; Wu, Y.-X.; **Yu, J.-L.**; et al. X-ray Structure-Guided Discovery of a Potent, Orally Bioavailable, Dual Human Indoleamine/Tryptophan 2,3-Dioxygenase (hIDO/hTDO) Inhibitor That Shows Activity in a Mouse Model of Parkinson's Disease. ***J. Med. Chem.*** 2021, 64, 8303-8332.